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Title: A DEVICE FOR WRITING THE TIME TAIL FROM SPALLATION NEUTRON PULSES

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A device for cutting the time tail from spallation neutron pulses

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ABSTRACT

The presence of long time tails in the neutron pulse produced by spallation sources is sometimes a problem in that it leads to background and can diminish the resolving power of the spectrometer. This problem is potentially severe with coupled moderators that are capable of providing increased intensity but at the cost of longer tails. The simple device we propose here is based on rocking a stack of multi-layers in the incident beam to attenuate these tails in a given band of incident wavelengths. The device and its operation are described and we present the results of Monte Carlo simulations.

Keywords: Spallation neutron source, pulsed beam, time-tail, tail-cutting, coupled moderator, multi-layer, protein crystallography, Monte Carlo, Los Alamos Neutron Science Center, chopper.

1.INTRODUCTION

Recent work at Los Alamos Neutron Science CEnter (LANSCE), has shown that there are large gains in neutron beam intensity to be made by using coupled moderators at spallation neutron sources.[1] Most of these gains result from broadening the pulse-width in time. However the accompanying longer exponential tail at large emission times can be a problem in that it introduces relatively large beam-related backgrounds at high resolutions. We have designed a device that can reshape the moderated neutron beam by cutting the time-tail so that a sharp time resolution can be re-established without a significant loss in intensity.

In this work the basic principles behind the tail-cutter and some initial results of Monte Carlo simulations are described. Unwanted neutrons in the long time-tail are diffracted out of the transmitted neutron beam by a nested stack of aperiodic multi-layers [2], rocking at the same frequency as the source. Nested aperiodic multi-layers have recently been used at X-ray sources [3] and as band-pass filters in quasi-Laue neutron experiments at reactor neutron sources [4]. Optical devices that rock in synchronization with a pulsed neutron beam are relatively new but are already under construction at LANSCE.[5] The tail-cutter described here is a novel concept that uses existing multi-layer technology in a new way for spallation neutrons. Coupled moderators in combination with beam shaping devices offer the means of increasing flux whilst maintaining a sharp time distribution.

A prototype device is being constructed for the protein crystallography station at LANSCE.[6] The protein crystallography station incorporates a water moderator that has been judiciously coupled in order to increase the flux over neutron energies that are important to structural biology (3-80meV).[1] This development in moderator design is particularly important because protein crystallography is flux limited and because conventional ambient water and cold hydrogen moderators do not provide relatively large neutron fluxes over this neutron energy range.

2. BASIC PRINCIPLE OF THE TAIL-CUTTER

Consider moving a multi-layer with periodic layer-spacing, d, in a pulsed neutron beam so that the Bragg angle, $\theta(t)$, changes with time over the duration of the neutron pulse and in synchronization with the pulse. Neutrons are diffracted out of the beam if they satisfy the diffraction condition given by;

$$\lambda(t-\tau)=2d\sin\theta(t)= (t-\tau)/(hL/m) \quad (1)$$

and when $\theta(t)$ is small

$$\lambda(t-\tau) \propto \theta(t) \quad (2)$$

where L is the distance from the moderator to the multi-layer, τ is the neutron emission time at the moderator, and t is the arrival time of neutrons at the multi-layer. The value of $\theta(t)$ is always relatively small for thermal neutrons because d is large, so, for a given τ, neutrons in a uniform range of wavelengths, $\lambda_{min} - \lambda_{max}$, can be diffracted from the beam by increasing $\theta(t)$ uniformly from a minimum, $\theta_{min} = \theta(t_{min})$, to a maximum, $\theta_{max} = \theta(t_{max})$, such that

$$\theta(t) = \theta_{min} + (t-t_{min})\Delta\theta/\Delta t \quad (3)$$

$$\lambda_{min} = (t_{min}-\tau)/(hL/m) \sim 2d\theta_{min} \quad (4)$$

$$\lambda_{max} = (t_{max}-\tau)/\ (hL/m) \sim 2d\theta_{max} \quad (5)$$

where $\Delta\theta$ is the angular range $\theta_{max}-\theta_{min}$ and $\Delta t = t_{max}-t_{min}$.

Now consider an aperiodic multi-layer, $d_{min}<d<d_{max}$. We can Bragg-reflect a finite range of neutron wavelengths, corresponding to a range of emission times, $\tau_{min} - \tau_{max}$, out of the incident beam at each angle, $\theta(t)$. For a given angle;

$$d_{min}/d_{max} = \lambda(t-\tau_{max})/\lambda(t-\tau_{min}) \quad (6)$$

The length of the time-tail to be cut will vary during the motion of the device. Values of τ_{min} and τ_{max} can be chosen so that all unwanted neutrons in the time-tail are diffracted out of the beam for all t, and only neutrons with $\tau<\tau_{min}$ are transmitted. Having determined the value of the ratio in (6) by selecting values for τ_{min} and τ_{max}, the values of d_{min} and d_{max} can be chosen. The value chosen for d_{max} is particularly important because it effectively determines $\Delta\theta$. By increasing or decreasing d_{max}, $\Delta\theta$ can be decreased or increased, respectively. Similarly, by increasing or decreasing L, $\Delta\theta$ can be decreased or increased, respectively. However, the lower limit of d_{max} is ultimately determined by the technical feasibility of producing multi-layers with the corresponding d_{min}.

Two factors that are likely to limit the effectiveness of this device are beam divergence and multi-layer quality. We can represent these factors by an effective angular resolution, $\delta\theta$. The maximum gain in time resolution without any loss of wanted neutrons can be represented by

$$\Delta\theta/\delta\theta = \Delta t/\delta t \quad (7)$$

where δt is the minimum possible time width and can be related to τ. By adjusting the phase lag of the device and allowing either some wanted neutrons to be diffracted or some unwanted neutrons to be transmitted the time width of the pulse can be finely tuned.

3. COUPLED VERSES DECOUPLED MODERATORS

The calculated pulse shapes at 2.4A at the moderator for a coupled, partially coupled, or decoupled water moderator are shown in Figure 1. Some of the main characteristics of these pulse shapes are given in Table 1. The lengthening of the tail as the moderator gets more strongly coupled is obvious from Figure 1. Of course the width of the main peak of the pulse, $\sigma_0(t)$, and the width of the time-tail, $\sigma_1(t)$, vary with wavelength, no matter what the moderator coupling scheme is. This is illustrated by Figure 2, which shows the calculated probability density of neutron emission as a function of neutron emission time and wavelength for the protein crystallography station water moderator at LANSCE. At best the time tails will introduce a background in adjacent time channels but at worst they will significantly diminish the resolving power of the spectrometer.

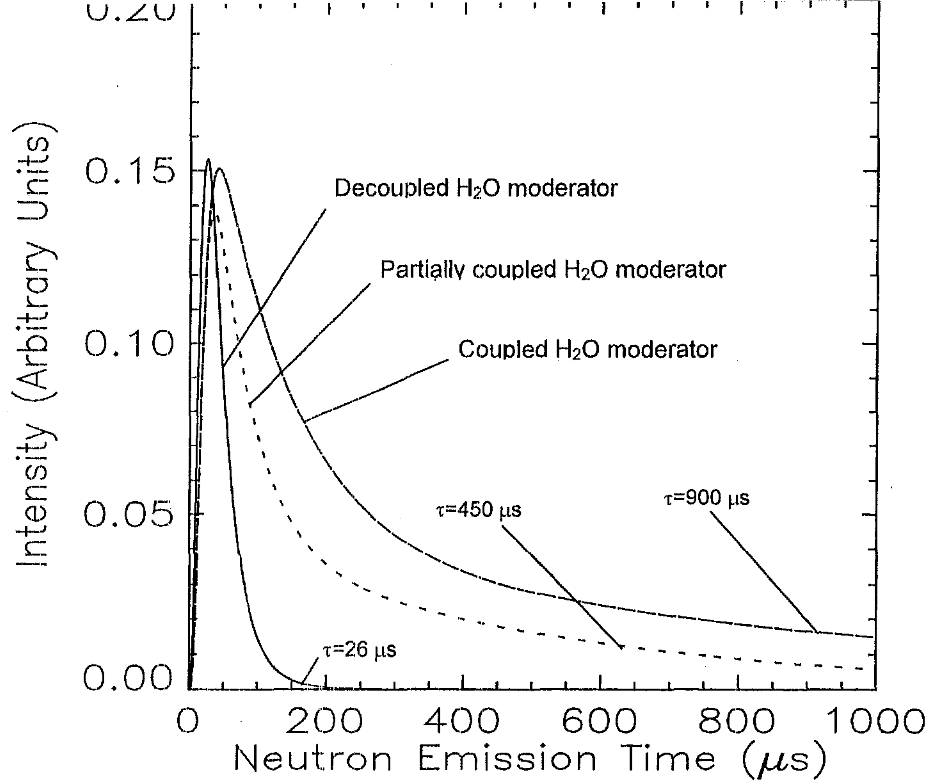

Figure 1: Pulse shapes at 14 meV for typical decoupled, partially coupled, and coupled moderators. moderator at the Los Alamos Neutron Science Center.

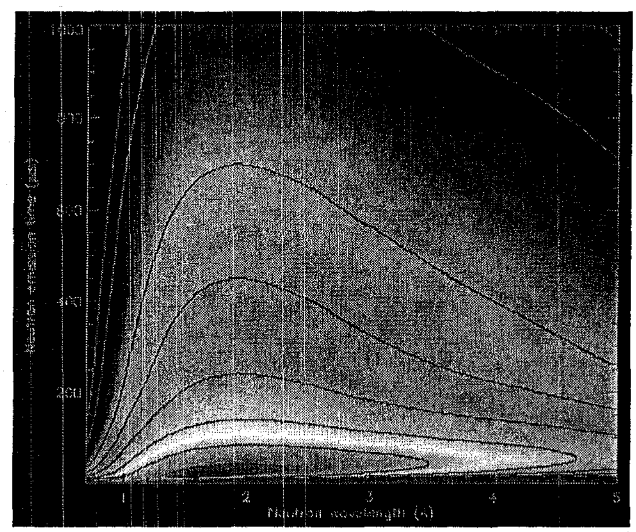

Figure 2 : Calculated emission time-wavelength distribution function for the Protein Crystallography Station (PCS) coupled water moderator.

The values of ratio (6) for the coupled and the partially coupled moderator are ~1/3 and ~2/3 respectively. A technologically conservative value for d_{min} would be 70A, leading to values of 200A and 105A for d_{max} for the coupled and partially coupled moderators, respectively. For a coupled moderator the device would travel at constant angular velocity over $\Delta\theta$ from 0.15° to 0.72°. For a partially coupled moderator the device would travel at constant angular velocity over $\Delta\theta$ from 0.3° to 1.4°. For the protein crystallography station $\delta\theta$=0.15°, corresponding to values of 0.263 and 0.136 for ratio (7). At 10m from the source Δt is 10ms, giving values for δt of 2.63ms and 1.35ms for the coupled and partially coupled moderators, respectively. At 5m from the source Δt is 5ms, giving values of δt of 1.32ms and 0.68ms for the coupled and partially coupled moderators, respectively. The improvement in time width can be represented by the ratio $\sigma_1/\delta t$. For

	Decoupled H_2O moderator	Partially coupled H_2O moderator	Fully (H_2O m
FWHM	41 μs	88 μs	15.
Standard deviation	32 μs	252 μs	26
(Relative) integrated intensity	1	3.5	5

Table I – Comparison of the basic characteristics of moderator time distributions at 14 meV (2.4 Angstrom).

a partially coupled moderator $\sigma_1/\delta t$ is ~2.9 at 5m and ~1.5 at 10m. For a coupled moderator $\sigma_1/\delta t$ is ~4.5 at 5m and ~2.3 at 10m. These values represent a very significant improvement in time resolution.

4.MONTE CARLO APPROACH

In order to investigate the time and energy distribution of neutrons transmitted by the rejecting device we have used a Monte Carlo computation approach.[7-8] When simulating the transmission of these pulses through the tail-cutter, the tail-cutter's properties have been modeled on those of easily fabricated Ni/Ti multi-layers. The d-spacings were conservatively chosen to start at 70A and increase linearly to 460A, although much smaller d-spacings are technologically feasible. A substrate thickness of 0.5mm was chosen although multi-layers have been deposited on much thinner silicon substrates. The nested stack of multi-layers is built up from 200 silicon wafer slides 100mm long, 0.5mm thick and with variable width, ω.Figure 3 shows a calculated reflectivity profile for a single Silicon wafer coated with 600 Ni/Ti bi-layers. This profile is used in our Monte Carlo simulations.

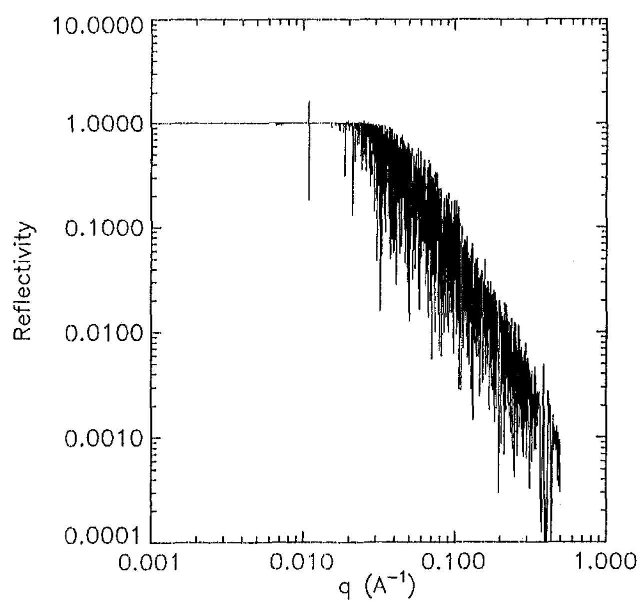

Figure 3: Calculated reflectivity profile for a single Si wafer coated with 600 Ni/Ti bilayers. The d-spacing of the structure increases linearly from d=70 A to d=460 A.

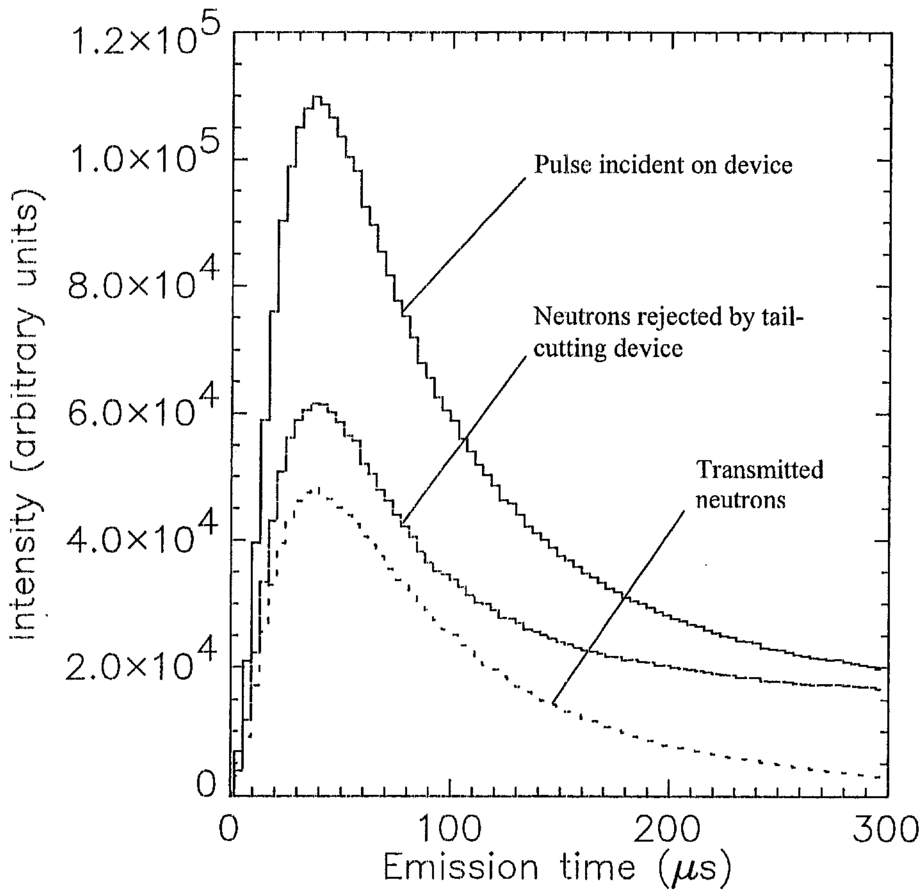

Figure 4a: Transmission of a pulse of 3 Angstrom neutrons through a tail-cutting device (Monte Carlo simulation). The device is phased so as to drastically reduce the exponential tail; the price paid is a significant reduction in intensity.

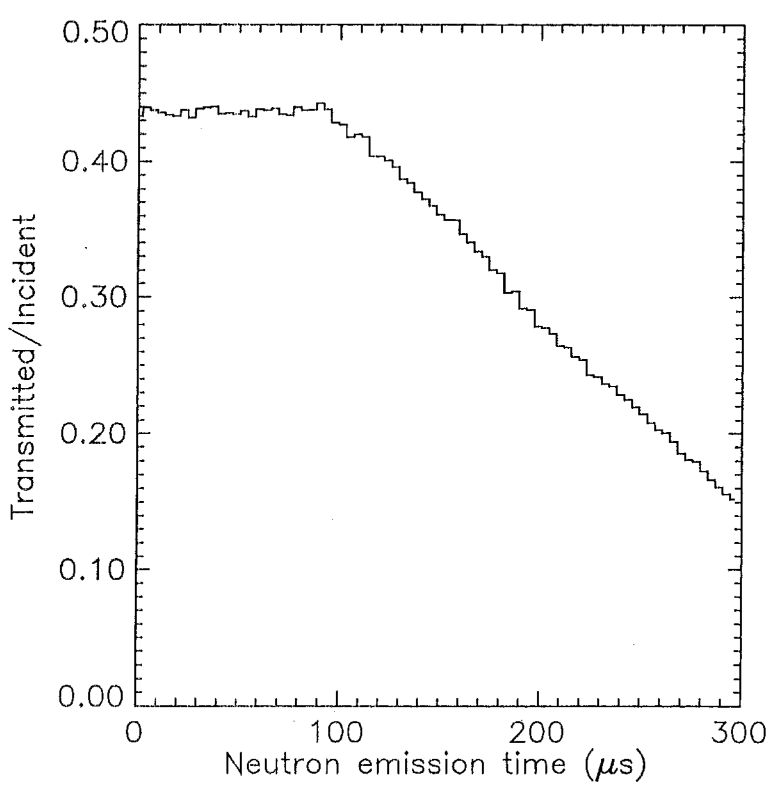

Figure 4b: Ratio of transmitted to incident pulse. Although the device attenuates the incident beam, the attenuation is clearly stronger for "tail" neutrons. About 45% of the intensity in the peak is transmitted while the tail is strongly attenuated.

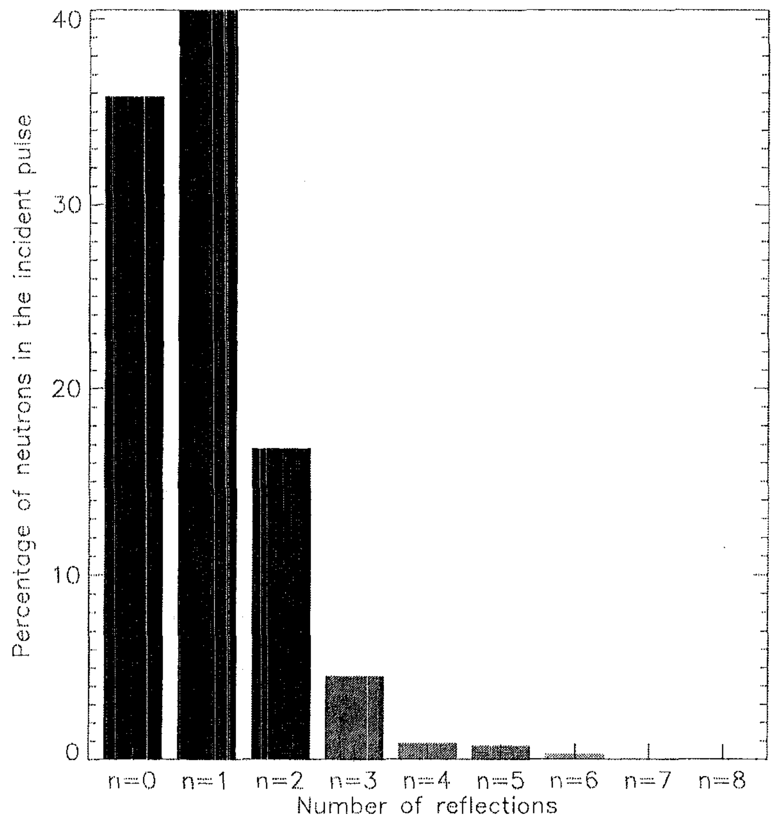

Figure 5: Transmission of a 3 Angstrom neutron pulse through a 3 cm thick device. About 36% of all incident neutrons (mostly in the peak) are transmitted; 41% of the neutrons (mostly in the tail) undergo one reflection and are removed from the transmitted pulse. This is a somewhat extreme situation where much intensity was sacrificed in order to drastically reduce the tail. In practice it is possible to phase the device to adjust the trade-off between tail reduction and transmitted intensity reduction.

The value of ω can be chosen so that at a particular θ all incident unwanted neutrons are rejected by single reflection. However this ideal value of ω changes over the range of θ. If a mean value of ω is used, then at some angles some unwanted neutrons will be transmitted without any reflection and at other angles some unwanted neutron will be transmitted by double reflection. After arriving at an optimum value for ω, we have investigated the effect of varying δt using the Monte Carlo methods. If the condition that no wanted neutrons are rejected is relaxed then the time resolution can be improved further at the expense of the neutron flux by decreasing the lag time, δt.

Figure 4a shows typical results for ω = 3 cm and 3 Angstrom neutrons –roughly in the middle of the 1-5 Angstrom bandwidth of interest. It is clear from Figure 3 that tail cutting comes at the expense of a reduction in intensity, which at first may appear severe. However, as shown in Figure 4b, which depicts the ratio of the transmitted to the incident pulse shape, it is clear that the tail is more dramatically reduced than the main peak. As pointed out above, it is possible to adjust the trade-off between intensity loss and tail reduction continuously.

The distribution of neutrons that pass through the device or make n=1, 2, 3, ... bounces is shown in Figure 5. More than 75% of all neutrons either pass through the device or make one bounce even with ω as large as 3 cm.

5. CONCLUSIONS

Our studies indicate that a rejecting tail-cutting device can reshape the time-width of a neutron pulse from a coupled or partially coupled moderator. For the Protein Crystallography station at LANSCE, the time width can be reduced by a factor of between 1.5 to 2.9 for a partially coupled moderator and by a factor of between 2.3 to 4.5 for a coupled moderator, with a decrease in the flux of the unwanted neutrons by ~95%. Double reflection results in some transmission of unwanted neutrons, but by judiciously optimizing the geometry of the device this can be kept below 5%. Even larger reductions in time width can be realized if a reduction in the flux of the wanted neutrons is acceptable. This pulse shaping device in combination with partially coupled or coupled water moderators allows the neutron flux over the intermediate wavelength range to be maximized whilst maintaining a narrow profile.

The parameters used in our proof-of-principle Monte Carlo studies were technologically conservative and the reflectivity profiles used for the silicon wafers were not ideal. The prototype device being constructed for the protein crystallography station at LANSCE has d-spacings increasing linearly from d=20A to 30A and will be positioned at 10m from the source. The tail cutter will be rocked at 20Hz from $\theta=1^\circ$ to 3.8°. The value of is δt 580μs with $\delta\theta$ around 0.2°. The thickness of the multi-layer substrate is 200μm.

An alternative method of shaping the time profile of a neutron pulse is to use a chopper. However in order for this to succeed the chopper has to be placed almost immediately after the moderator. The large amounts of shielding and reflecting material that must be placed around moderators would make such a chopper hard to access and maintain. The Rejecting device presented here offers a cheap alternative that is easy to access and maintain.

The Rejecting device could be applicable to other types of neutron spectrometer where the time profile of the neutron pulse has to be tailored. Perhaps the greatest potential application would be with spectrometers on long-pulse spallation neutron sources, where the time width is relatively large.

In addition to the Rejecting device there is also the possibility of a Selecting device. Such a device would require two parallel nested aperiodic multi-layer stacks rocking in synchronization, so that wanted neutrons are diffracted out of the beam and then directed along a parallel direction by double reflection.

ACKNOWLEDGEMENTS

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